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Methanol Synthesis from Renewable Electrical Energy: A Feasibility Study

M. Rivarolo[*], D. Bellotti, L. Magistri

Thermochemical Power Group, University of Genoa, 1 Via Montallegro Str., 16145 Genova Italy

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This paper aims to present a feasibility study of an innovative plant for methanol synthesis from carbon dioxide and hydrogen, produced by water electrolyser fed by renewable electrical energy. The analysis aims to examine a methanol production plant, based on 1MW of installed electrolyser, from both the management and economic standpoints: the 1MW plant size has been chosen to represent a modular plant for the power to fuel distributed generation, which may be powered by renewable energy.

The thermo-economic investigation is performed using two different approaches: a detailed design point analysis, carried out in order to identify the optimal component sizes and operating parameters followed by a time-dependent plant management optimization.

Both the studies are carried out with two simulation tools, named WTEMP (Web-based Thermo-Economic Modular Program) and W-ECoMP (Web-based Economic Poly-generative Modular Program), both developed by the Thermochemical Power Group at University of Genoa.

Key words: power to fuel, thermo-economic analysis, methanol production.

INTRODUCTION

According to recent evaluations, world energy demand is expected to increase significantly by 2050: despite fossil fuels will be still the predominant primary source, renewable energy sources (RES) contribution is expected to increase as well 1. At the same time, European Countries are investigating innovative systems in order to reduce CO_2 emissions developing new kind of fuels (i.e. biofuels), which have low carbon footprint for the energy production. On the other hand, the increasing RES penetration, in particular in case of not fully controllable sources as solar and wind, introduces new issues in terms of electrical system management and energy balance: in particular, the wide exploitation of not predictable and storable RES which have the priority in the energy market, has recently caused significant troubles to traditional power plants (i.e. combined cycles), forcing them to operate in strong off-design conditions at lower efficiencies, with numerous on/offs that affect negatively the plant lifetime and pollutant emissions.

The power-to-fuel (PtF) technologies seem to represent a good solution in this sense, allowing to absorb electrical energy (i.e. RES overproduction), converting and storing it into chemical form, for example for the production of biofuels.

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[*] To whom all correspondence should be sent:
E-mail: massimo.rivarolo@unige.it

however, with this method, about 0.6-1.5 tons of CO2 are emitted for each ton of produced methanol 45. This paper analyzes an alternative and sustainable method for methanol production: methanol is synthesized from a mixture of hydrogen and carbon dioxide. The hydrogen is produced by water electrolysis employing renewable electrical energy, while CO2 is sequestrated from the flue gas of a fossil power plant 67. The reaction is reported below:

$$CO_2 + 3H_2 \leftrightarrow CH_3OH + H_2O \qquad (1)$$

The catalytic reaction takes place in ranges of temperature and pressure of 250 – 300 °C and 50 - 100 bar, respectively on CuO/ZnO/Al2O3 as catalyzer 89.

The study is performed using two different software, both developed by the authors' research group at University of Genoa, named respectively WTEMP (Web-based Thermo-Economic Modular Program) and W-ECoMP (Web-based Economic Cogeneration Modular Program).

WTEMP allows the thermos-economic analysis of a large number of energy systems (steam plants, gas turbines, combined cycles, power to fuel systems, biomass gasification, fuel cells, etc.). Some components of energy systems can be studied, previously, varying operative conditions by Impedance Spectrocopy [10,11], that is is a valuable tool for the investigation of reactions and phenomena taking place in different materials [12-177]. Operating characteristics and mass and energy balances of each component, in the on-design state, are calculated sequentially until the conditions (pressure, temperature, mass flow, etc.) at all interconnections converge on a stable value. After the thermodynamic calculation, the thermo-economic analysis is performed: at first each component purchase cost is defined through the use of cost or costing equations, therefore the internal thermo-economic and exergoeconomic analysis is carried out through the cost and exergy balances of each module 18.

W-ECoMP is a software which aims to the management strategy optimisation, minimizing a target function which is rapresentative of the annual costs of the plant; the optimization process is based on a genetic algorithm. Compared to WTEMP, W-ECoMP is a software that performs a time-dependent thermo-economic analysis, usually by dividing the operational time (usually a year) with sufficient number of representative periods (one hour or less depending on the particular application) 18.

The first step for the economic analysis is the calculation of the Purchased Equipment Cost (PEC), which is determined on the basis of the cost funtions of the different components of the plant under analysis. Starting from the PEC, it is possible to calculate the Total Capital Investment (TCI), taking into account different costs depending on the economic scenario where the plant is operating (i.e. construction and installation costs, the start-up cost, working capital, licensing, allowance etc). The final aim of the analysis is the calculation of the investment's profitability in order to choose the best solution, taking into account the initial investment and the associated risks related to the economic scenario and to the characteristic of the plant.

More details about W-ECoMP can be found in other authors' publications 192021.

THERMODYNAMIC ANALYSIS

Before performing the economic analysis, a thermodynamic analysis is necessary in order to define the operating parameters of the plant. The mass flows, the electrical consumption and the thermal energy input and output must be defined for each plant component in order to understand the mutual interaction between the different parts of the system. The PtF plant under investigation is composed by three main components:

- Carbon capture system (CCS): the CCS is connected to the coal-fired power plant and sequestrates, the CO_2 required by the methanol production process, from the flue gases;
- Water electrolyser: this device employs electrical energy to produce, by water electrolysis, the hydrogen for the methanol synthesis; furthermore a significant amount of oxygen (about 8 times the hydrogen, in mass terms) is co-produced by the process;
- Methanol reactor: the mixture of hydrogen and carbon dioxide is sent to the reactor for the methanol production, according to Equation (1).

The simplified scheme of the plant is reported in Figure.1.

In order to produce the so called "green methanol", only renewable generators are considered for the electrolyser energy supply. To this aim, different renewable energy sources, such as solar and wind, are taken into account. Moreover, different management options (only solar, only wind or a combination of both) are analyzed in order to define the best solution from both the economic (based on costs-revenues and on the total capital investment) and the operating point of view (based on the utilization factor and the exploitation rate of the RES).

The thermodynamic analysis is performed using the WTEMP software, described above. Several technical data are necessary for the characterization of each module of the plant to perform the thermodynamic analysis. All the data assumed for the simulations are reported below; in this analysis, most of the data are taken from literature or from real commercial data.

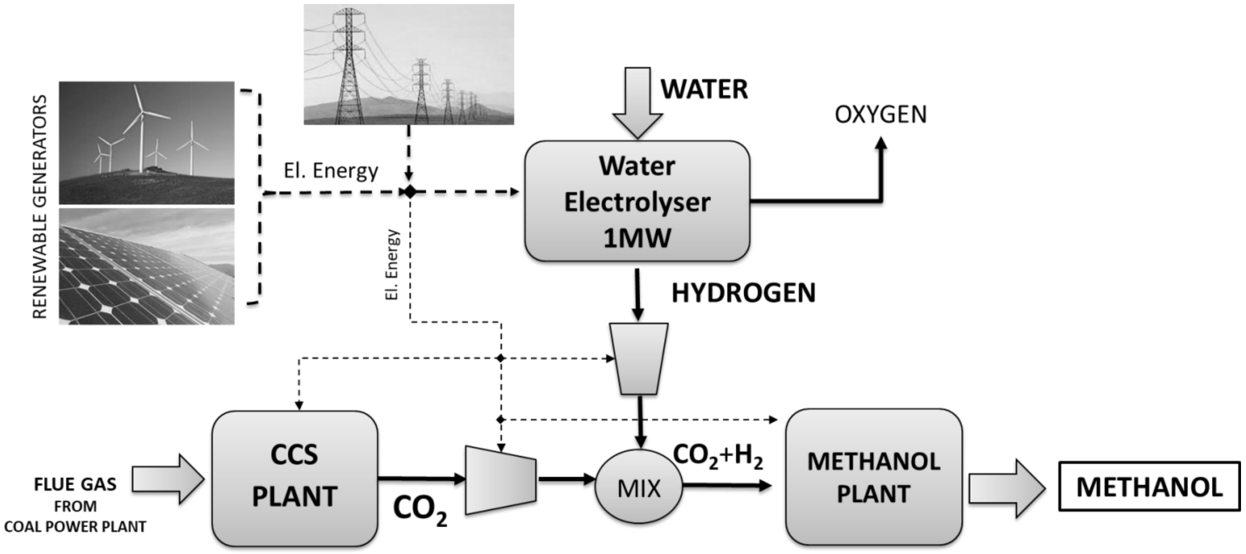


Fig. 1. Reference plant scheme

Table 1. Thermodynamic main assumption

AEC Electrolyser	
Electrical consumption	4.7 kWh/Nm^3 H_2
Pressure	30 bar
Temperature	80 °C
Efficiency	68%
Carbon Capture system	
Treatment kind	Amines MEA (30%)
Flue gases inlet T[°C] and p[bar]	40°C, 2bar
Thermal energy consumption per ton of CO_2	3 GJth/kgCO2
CO_2 outlet temperature[°C] pressure[bar]	40°C, 2 bar
CO_2 capture rate	90%
Methanol Reactor	
Working Pressure	80 bar
Temperature	240 °C
Recirculation factor of unreacted syngas	0.85
Conversion efficiency	96%
Molar H_2:CO_2 ratio	3:1

The reference plant size is based on 1MW of installed electrolyser: on the base of the parameters reported in Table 1, the electrolyser produces about 19kg/h of hydrogen and 151kg/h of oxygen (H_2:O_2 mass ratio is 8). Considering the stoichiometric methanol reaction, for 19kg/h of hydrogen, about 140kg/h of CO_2 are needed: the CCS system is sized in order to be able to produce that amount of CO_2, meaning that it is able to process about 824kg/h of flue gases, assuming a CO_2 average content equal to 17%.

The CO_2 exits the CCS section at 2bar; consequently it is pre-compressed up to 30bar before being mixed with the hydrogen. Then, hydrogen and carbon dioxide are mixed together and compressed to the reactor working pressure, equal to 80bar. In the table 2 below, the results of the thermodynamic analysis, in terms of mass flows, electrical energy consumption and thermal energy input and output, are summarized.

It is worth noting that the largest energy consuming component of the plant is the AEC (1MW installed), the energy demand of the other components (about 30 kWh in total) is just the 3% of the total demand and therefore it results considerably lower compared to the electrolyser demand.

Table 2. Thermodynamic simulation main results

AEC Electrolyser	
Power installed	1MW
Hydrogen outlet	19 kg/h
Oxygen outlet	152 kg/h
Water consumption	195 kg/h
CCS system	
Flue gas in	823 kg/h
wt% CO_2 in flue gas	17%
CO_2 out	140kg/h
Thermal energy consumption	117 kWh_{th}
Electrical energy consumption	7 kWhe
Methanol reactor	
Mixture inlet	159kg/h
Methanol outlet	97 kg/h
Thermal energy outlet	31kWh_{th} (based on the heat of reaction)
Compressors	
CO_2 compression (from 2 up to 30 bar)	9.8 kWh
H_2 + CO_2 compression (from30 up to 80 bar)	13 kWh

THERMO-ECONOMIC ANALYSIS

The thermo-economic analysis aims to study a reference methanol production plant, based on 1MW of installed electrolyser, from both the management and economic point of view. For simplicity, the 1MW plant size has been chosen to represent a modular plant for the PtF distributed generation, which may be powered by RES. In the following, the influence of the plant size on the economic feasibility will be presented. First, in order to analyze the production process of 100% green methanol, the direct coupling of different RES plants (wind, solar or a combination of the two), to the methanol plant is investigated.

Main assumptions

The RES under analysis are the solar energy (using PV panels), wind energy or a combination of both. In order to simulate the energy production from RES, it is necessary to extrapolate the solar insulation curve and the wind velocity curve from the database available for the area near to the installation site. In the Figure 2 average monthly solar irradiation is reported: each curve represents the trend in a typical day representative of the month. The magnitude of the curves changes during the year, following the seasons.

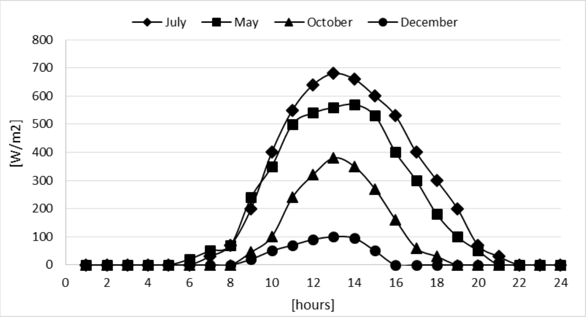


Fig. 2. Average monthly solar irradiation [22]

In Figure 3, the values of the wind velocity hour by hour are reported; in this case it is not possible to recognise a specific profile because the values are completly stochastich. It is just possible to identify an average trend season by season.

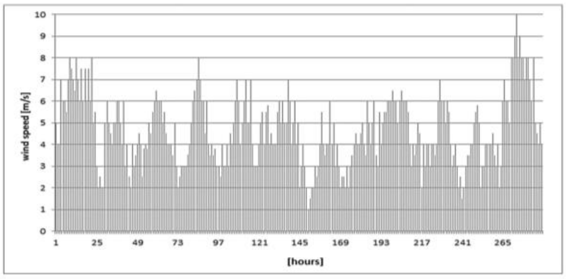


Fig. 3. Wind velocity profile [23]

To perform the analysis, the German economic scenario is chosen and the following economic assumptions are considered:

Methanol selling price is assumed to be 400 €/ton, that is the average market price between 2014 and 2015 in Europe, as reported in 24;

Oxygen selling price highly depends on its diffusion on the market, which is related to local conditions, applications, etc. In the case under analysis, oxygen price is assumed 100 €/ton, which represents the minimum selling price for industrial use of oxygen (rates are higher for medical use). It is worth noting that the purity of oxygen produced by electrolysers (>99.9%) is sufficient for industrial applications, therefore no further purification treatments are needed;

Electrical energy cost represents a term of primary importance to determine optimal system configuration. The electrical energy to feed electrolysers is produced by renewable sources that are strongly variable hour by hour and it is not always available to feed the system at the nominal conditions. When the renewable energy is not available and it is assumed to operate at nominal conditions, the electrical energy is purchased from the grid. The average energy cost is assumed equal to 0.037€/kWh that is the market value for 5 MW maximum installed plant in Germany 25;

Electrical energy selling price: the possibility of selling the surplus (respect the methanol plants demand) energy produced by the renewable sources is also taken into account. The market price of renewable energy sold to the grid is assumed equal to 0.073 €/kWh, which is the incentivized price for RES producers in Germany (at 2014) 25;

Capital cost: In order to calculate the TCI is necessary define the PEC that is the sum of the capital cost of the each component of the plant (electrolyser, CCS system and methanol reactor). The capital costs depend on the size and operating parameters of the component, the cost functions used for this analysis are reported in Table 3 below.

Plant lifetime is assumed equal to 15 years to be conservative, considering the lifetime of the electrolysers, which is the most expensive plant component;

Methanol plant equivalent operating hours is assumed equal to 8640 hours per year, which represents a typical value for this kind of plants: in fact, due to the great inertia of chemical reactors, the methanol plant should operate at nominal conditions for the whole year, if possible:

Inflation is assumed equal to 0.4 %, which represents a typical value in Germany, Figure 4 [26].

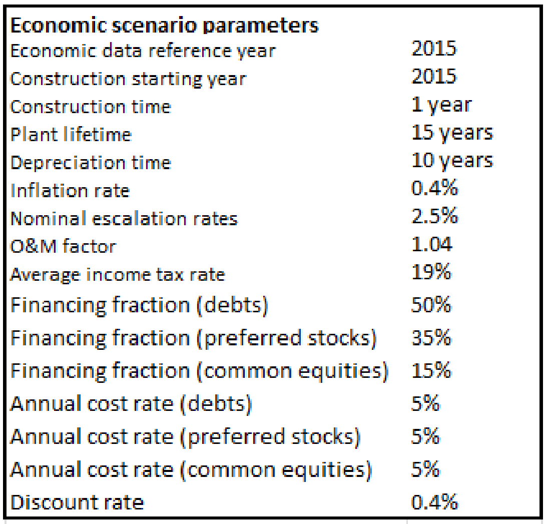
Average income tax rate is assumed equal to 19%, which is a typical value in Germany 26.

Tab. 4 reports the main data assumed for the present thermo-economic analysis. All these data are inputs for the W-ECoMP software.

Table 3. Thermodynamic simulation main results

Plant component	Cost function	
Pressurized electrolyser	$C_{AEC} = 1.3 \cdot 10^6 \cdot P[kW]^{0.815}$	[€]
CCS plant (CO_2 separation)	$C_{CCS} = 75.45 \cdot 10^6 \left(\frac{M_{in}\left[\frac{kg}{h}\right]}{2.808 \cdot 10^6} \right)^{0.65}$	[€]
Methanol reactor	$C_{MeOH} = 14.2 \cdot 10^6 \left(\frac{M_{in}[kg/h]}{54000} \right)^{0.65}$	[€]
PV panels	$C_{PV} = 2000 \cdot P[kW]$	[€]
Wind generator	$C_{wind} = 1500 \cdot P[kW]$	[€]

Table 4. Economic data



Economic scenario parameters	
Economic data reference year	2015
Construction starting year	2015
Construction time	1 year
Plant lifetime	15 years
Depreciation time	10 years
Inflation rate	0.4%
Nominal escalation rates	2.5%
O&M factor	1.04
Average income tax rate	19%
Financing fraction (debts)	50%
Financing fraction (preferred stocks)	35%
Financing fraction (common equities)	15%
Annual cost rate (debts)	5%
Annual cost rate (preferred stocks)	5%
Annual cost rate (common equities)	5%
Discount rate	0.4%

Cases description

In this preliminary thermo-economic analysis, it is assumed to integrate the methanol plant with different RES (solar and wind). Considering the stochastic nature of RES, the renewable generators have been oversized in order to have an acceptable amount of energy supply. Three different plant configurations, based on the RES employed, are investigated keeping constant the size of the electrolyser (1 MW):

Case 1: 3MW of PV panels installed.

The PV panels are installed to generate the energy necessary to the hydrogen production by water electrolysis. When the renewable source is not available, the electrical energy is purchased from the grid in order to ensure the AEC electrolyser to work at the nominal conditions. The system works at the rated condition imposed by the size of the electrolyser.

Case 2: 3MW of wind generator.

Wind turbines are installed to generate hydrogen by water electrolysis and to produce the required hydrogen, when the renewable source is not available the electricity is purchased by the national grid to help stabilize the hydrogen production. The system works at the rated condition imposed by the size of the electrolyser.

Case 3: 1.5MW of PV panels and 1.5MW of wind generator installed.

This case is similar to the previous configurations, but both PV field and wind farm are installed and interconnected to generate hydrogen by water electrolysis. The possibility to interconnect the two renewable sources is analyzed to increase the periods in which renewable energy is provided. Consequently, the percentage of green methanol (defined as the methanol produced employing only renewable energy) is increased. When renewable sources are not available the electricity is purchased from the national grid.

For each of the three Cases described above, two different energy options are taken into account:

A: The PtF is only fed by the renewable energy (production of “100%” green methanol)

B: The PtF is fed by the renewable energy, when available, and by grid energy in the other periods.

It is worth underling that this is a theoretical analysis that aims to investigate the possibility of coupling a renewable plant directly to the PtF plant from both the operating and economic point of view in order to identify any critical aspects that can be improved with further development.

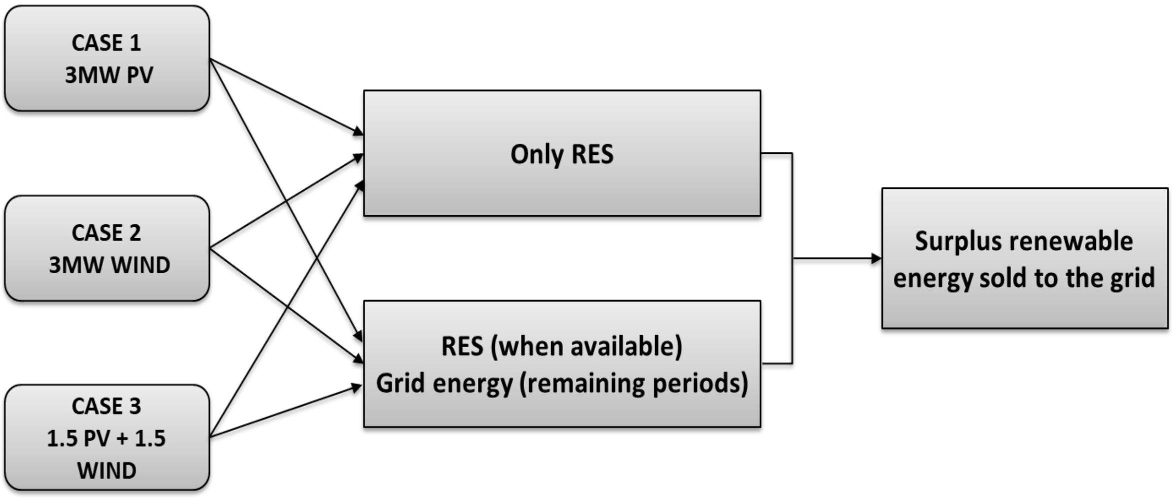


Fig. 4. Scheme of the different cases under analysis

MAIN RESULTS

In this thermo-economic analysis, the management option *A* for the three different plant configurations is investigated from an operating and economic point of view. It is assumed to feed the methanol plant employing only the renewable energy produced by 3MW renewable power plant that is represented by PV panels (case 1), wind generator (case 2), integration of both (case 3).

In Table 5 a comparison between the three cases from the operating point of view is reported: it is evident that the case 2A is the best solution because it presents the highest renewable energy production and the highest utilization factor as well. This entails a higher methanol production and therefore higher revenues as reported in Figure 6.

Figure 5 shows that the Case 2A results the best solution also from the economic point of view: although the system is not profitable due to the high costs value, it has the minimum difference between the cost and revenues due to the combined effect of higher revenues and lower TCI.

In the second part of the analysis, the management option B for three different plant configurations is investigated as well: it is assumed to feed the methanol plant employing, when available, the renewable energy produced by 3MW generators, represented by PV panels (case 1), wind generator (case 2) or integration of both (case 3). In the remaining periods, the electrical energy is purchased from the grid in order to keep the methanol plant at constant nominal conditions.

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Table 5. Operating management comparison (case A)

		CASE-1A (3MW PV)	CASE-2A (3MW WIND)	CASE-3A WIND + PV
Total Energy production	[MWh]	4800	7004	5902
Equivalent hours	[h]	1600	2335	1203
RES energy to AEC	[MWh]	3026	5123	4699
AEC utilization factor	[%]	34	57	53
RES energy to the grid	[MWh]	1774	1881	1190
Methanol production	[ton]	295	494	458

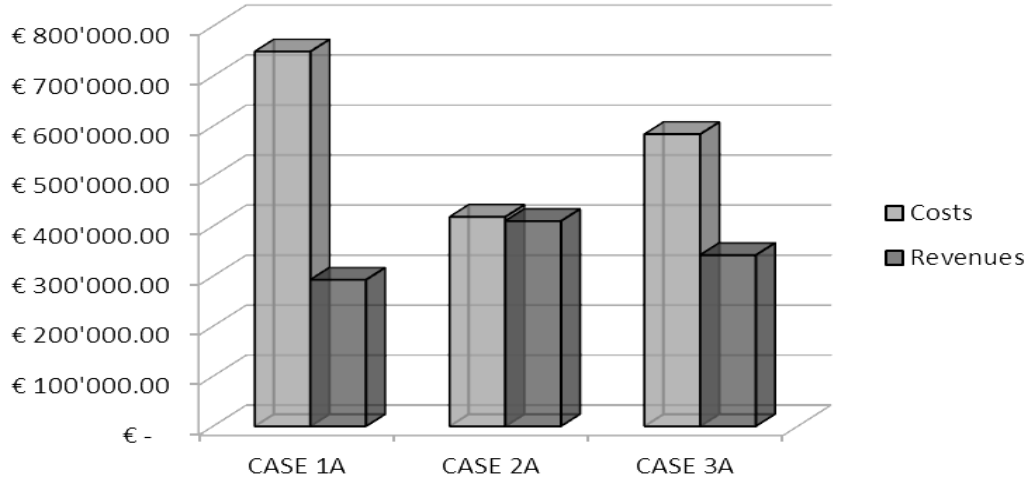

Fig. 5. Case comparison: costs and revenues

In Table 6 a comparison between the three cases from the operating point of view is reported: it is evident that the case 2B results again the best solution because of the highest amount of renewable energy utilized by the plant and consequently the lowest amount of purchased energy. Moreover, it presents also the highest amount of surplus renewable energy that can be sold to the grid. For these reasons, together with the lower TCI (due to the lower capital cost of the wind generator than the PV panels), the case 2B represents the best solution also from the economic point of view and the only one with a positive balance between costs and revenues, as shown in Figure 6.

Table 6. Operating management comparison (case B)

		CASE-1B (3MW PV)	CASE-2B (3MW WIND)	CASE-3B (1.5 PV + 1.5 WIND)
Tot. Energy production	[MWh]	4800	7004	5902
Equivalent hours	[h]	1600	2335	1967
Renewable energy to AEC	[MWh]	3026	5123	4699
AEC utilization factor	[%]	100	100	100
El. energy purchased from grid	[MWh]	5904	3807	4231
RES energy sold to the grid	[MWh]	1774	1881	1190
Methanol production	[ton]	866	866	866

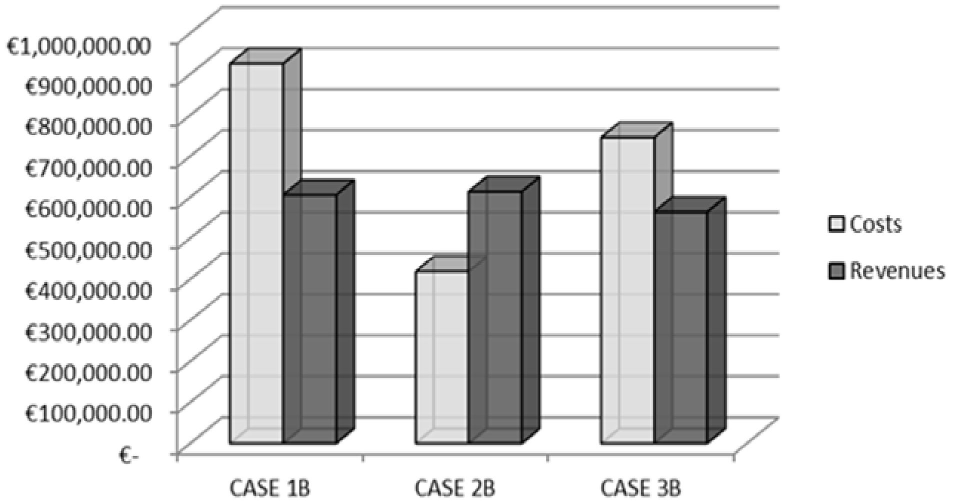

Fig.6. Costs and revenues comparison (case B)

CONCLUSION

In the paper, RES and methanol plant integration has been investigated. Three different plant configurations have been taken into account on the basis of the typology of RES coupled to the plant: in configuration 1 it was assumed to install 3MW of PV panels, in configuration 2 it was assumed to install 3MW of wind generators and, in configuration 3, the interaction between the two different energy sources was investigated: the 3MW of renewable power installed was distributed equally between PV panels (1.5MW) and wind generator (1.5MW).

Each configuration was analyzed considering two different energy options: (A) feeding the system with RES only; (B) powering the plant with RES, when possible, and purchasing the electrical energy from the grid in the remaining periods The following considerations can be drawn:

- Taking into account the energy option A, the system is forced to operate under discontinuous conditions: the utilization factor results significantly reduced; moreover this operating strategy would not be compatible with the methanol reactor.
- Taking into account the option B, the plant can operate continuously at nominal condition, the methanol production increase up to the 100% of the capacity plant; on the other side the electricity purchased increases the operating costs and the methanol produced is not "*100% green*".
- The solar energy source presents a high rate of predictability that allows the system to operate in on-off modality with a regular profile; on the other hand, PV panels present a lower energy production compared to the wind generators.
- The best solution results to be the configuration 2B: since renewable energy production is higher, the green methanol produced results the highest as well as the amount of surplus energy sold to the grid. Moreover, wind generators capital cost are lower than the PV panels: thus, configuration 2B results the best one also from the economic standpoint.

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Nomenclature

AEC	Alkaline Electrolyser
CCS	Carbon Capture Sequestration
PEC	Purchased Equipment Cost
PtF	Power to fuel
RES	Renewable Energy Sources
TCI	Total Capital Investment
TPG	Thermochemical Power Group
WTEMP	Web-based Thermo-Economic Modular Program
W-ECoMP	Web-based Economic Cogeneration Modular Program

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Синтез на метанол от възобновяема електрическа енергия: Предпроектно проучване

М. Риваролo *, Д. Белоти, Л. Магистри

Група по термомеханика, Университет на Генуа, ул. Виа Монтенегро 1, 16145 Генуа, Италия

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(Резюме)

Тази статия представя предпроктно проучване на потенциала за осъществимост на инновативна инсталация за синтез на метанол от въглероден двуокисид и водород, произведен от електролизьор чрез възобновяема електрическа енергия. Анализът има за цел да представи инсталация за производство на метанол, базирана на инсталиран електролизьор с мощност от 1МВ, както от гледна точка на управление, така и от икономическа гледна точка: мощността на инсталацията от 1МВ е подбрана так, че да представлява модулна инсталация за разпределение на енергия произведена от възобновяеми енергиини източници.

Термо-икономическото изследване е осъществено като се прилагат два различни подхода: подробен анализ на проектните точки, осъществен с цел да се идентифицират оптималните размери на компонентите и оперативните параметри, последвани от оптимизация на управлението на инсталацията по време. И двете проучвания са осъществени с две методики на симулация, наречени ВТЕМП (уеб-базирана термо-икономична модулна програма) и В-ЕкоМП (уеб-базирана икономична поли-генеративна модулна програма) разработени от групата по термомеханика към Университета в Генуа.